OpenCMISS-iron examples and tests used by OpenCMISS developers at University of Stuttgart, Germany

Christian Bleiler, Andreas Hessenthaler, Thomas Klotz, Aaron Krämer, Benjamin Maier, Sergio Morales, Mylena Mordhorst, Harry Saini

> July 4, 2017 16:11

CONTENTS

1	Introduction	3		
	1.1 Cmgui files for cmgui-2.9	3		
	1.2 Variations to consider	3		
	1.3 Folder structure	4		
2	How to work on this document			
3	Diffusion equation	5		
_	3.1 Equation in general form	5		
4	Linear elasticity	6		
	4.1 Equation in general form	6		
5	Finite elasticity			
6	Navier-Stokes flow			
7	Monodomain	9		
,	7.1 Example-0401	10		
	7.1.1 Mathematical model	10		
	7.1.2 Computational model	10		
	7.1.3 Results	11		
	7.1.4 Validation	11		
8	CellML model	11		

LIST OF FIGURES

^{*} Institute of Applied Mechanics (CE), University of Stuttgart, Pfaffenwaldring 7, 70569 Stuttgart, Germany

[†] Lehrstuhl Mathematische Methoden für komplexe Simulation der Naturwissenschaft und Technik, University of Stuttgart, Allmandring 5b, 70569 Stuttgart, Germany

[‡] Institute for Parallel and Distributed Systems, University of Stuttgart, Universitätsstraße 38, 70569 Stuttgart, Germany

Figure 1	Results movie, 24×24 elements (only works in cer-					
	tain pdf viewers, e.g. Adobe Acrobat Reader)	11				
Figure 2	Results, 10×10 elements, $t = 200 \dots \dots$	12				
Figure 3	Results, 24×24 elements, $t = 200 \dots \dots$	12				
Figure 4	Results, 24×24 elements, $t = 500 \dots \dots$	13				
LIST OF TABLES						
Table 1	Initials of people working on examples, in alphabetical order (surnames)	4				

1 INTRODUCTION

This document contains information about examples used for testing *OpenCMISS-iron*. Read: How-to¹ and [1].

- 1.1 Cmgui files for cmgui-2.9
- 1.2 Variations to consider
 - Geometry and topology

1D, 2D, 3D

Length, width, height

Number of elements

Interpolation order

Generated or user meshes

quad/hex or tri/tet meshes

- Initial conditions
- Load cases

Dirichlet BC

Neumann BC

Volume force

Mix of previous items

- Sources, sinks
- Time dependence

Static

Quasi-static

Dynamic

Material laws

Linear

Nonlinear (Mooney-Rivlin, Neo-Hookean, Ogden, etc.)

Active (Stress, strain)

- Material parameters, anisotropy
- Solver

Direct

Iterative

Test cases

Numerical reference data

Analytical solution

• A mix of previous items

¹ https://bitbucket.org/hessenthaler/opencmiss-howto

1.3 Folder structure

TBD..

HOW TO WORK ON THIS DOCUMENT

In the Google Doc at https://docs.google.com/spreadsheets/d/1RGKj8vVPqQ-PH0UwMX_ e9TAzqaYavKi0z0D4pKY9RGI/edit#gid=0 please indicate what you are working on or if a given example was finished

- no mark: to be done
- x: currently working on it
- xx: done

Initials	Full name
СВ	Christian Bleiler
AH	Andreas Hessenthaler
TK	Thomas Klotz
AK	Aaron Krämer
BM	Benjamin Maier
SM	Sergio Morales
MM	Mylena Mordhorst
HS	Harry Saini

 Table 1: Initials of people working on examples, in alphabetical order (surnames).

3 DIFFUSION EQUATION

3.1 Equation in general form

The governing equation is,

$$\partial_t \mathbf{u} + \nabla \cdot [\boldsymbol{\sigma} \nabla \mathbf{u}] = \mathbf{f}, \tag{1}$$

with conductivity tensor $\boldsymbol{\sigma}.$ The conductivity tensor is,

- defined in material coordinates (fibre direction),
- diagonal,
- defined per element.

4 LINEAR ELASTICITY

4.1 Equation in general form

$$\label{eq:delta_theta_$$

5 FINITE ELASTICITY

7 MONODOMAIN

7.1 Example-0401

7.1.1 Mathematical model

We solve the Monodomain Equation

$$\sigma \Delta V_{m}(t) = A_{m} \left(C_{m} \frac{\partial V_{m}}{\partial t} + I_{\text{ionic}}(V_{m}) \right) \quad \Omega = [0, 1] \times [0, 1], \quad t \in [0, 3.0]$$
(3)

where $V_m(t)$ is given by the Hodgkin-Huxley system of ODEs with boundary conditions

$$V_{m} = 0 x = y = 0, (4)$$

$$V_{m} = 0 x = y = 1. (5)$$

and initial values

$$V_{\rm m}(t=0) = -75$$

Additionally a stimulation current I_{stim} is applied for $t_{\text{stim}} = [0, 0.1]$ at the center node of the domain (i.e. at $(x, y) = (\frac{1}{2}, \frac{1}{2},)$).

Material parameters:

$$\sigma = 3.828$$

$$A_{\rm m} = 500$$

 $C_m = 0.58$ for the slow-twitch case, $C_m = 1.0$ for the fast-twitch case

 $I_{Stim} = 1200$ for the slow-twitch case, $I_{Stim} = 2000.0$ for the fast-twitch case

7.1.2 Computational model

- This example uses generated meshes
- Commandline arguments are:

number elements X

number elements Y

interpolation order (1: linear; 2: quadratic)

solver type (o: direct; 1: iterative)

PDE step size

stop time

output frequency

CellML Model URL

slow-twitch

ODE time-step

- Commands for tests are:
 - ./folder/src/example 24 24 1 0 0.005 3.0 1 hodgkin_huxley_1952.cellml F 0.0001
 - ./folder/src/example 24 24 1 0 0.005 3.0 1 hodgkin_huxley_1952.cellml F 0.005
 - ./folder/src/example 10 10 1 0 0.005 3.0 1 hodgkin_huxley_1952.cellml F 0.0001

mpirun -n 2 ./folder/src/example 24 24 1 0 0.005 3.0 1 hodgkin_huxley_1952.cellml

mpirun -n 8 ./folder/src/example 24 24 1 0 0.005 3.0 1 hodgkin_huxley_1952.cellml ./folder/src/example 2 2 1 0 0.005 3.0 1 hodgkin_huxley_1952.cellml F 0.0001 mpirun -n 2 ./folder/src/example 2 2 1 0 0.005 3.0 1 hodgkin_huxley_1952.cellml F

• This is a dynamic problem.

7.1.3 Results

Passed tests: 6 / 6

No failed tests.

Figure 1: Results movie, 24×24 elements (only works in certain pdf viewers, e.g. Adobe Acrobat Reader)

7.1.4 Validation

We compare with a Matlab implementation.

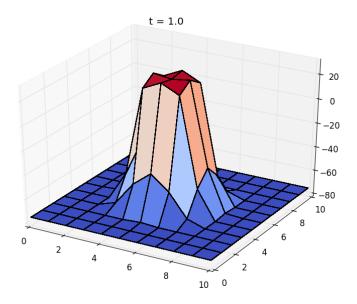


Figure 2: Results, 10×10 elements, t = 200

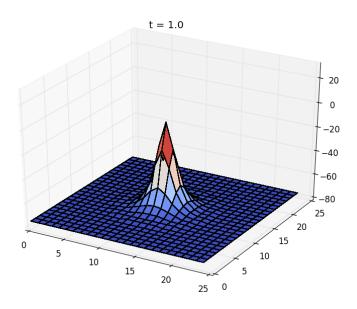


Figure 3: Results, 24×24 elements, t = 200

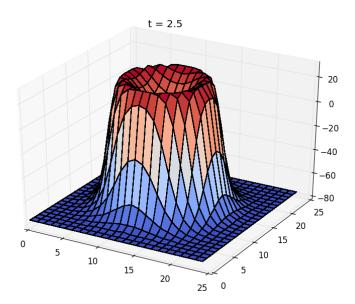


Figure 4: Results, 24×24 elements, t = 500

8 CELLML MODEL

REFERENCES

[1] Chris Bradley, Andy Bowery, Randall Britten, Vincent Budelmann, Oscar Camara, Richard Christie, Andrew Cookson, Alejandro F Frangi, Thiranja Babarenda Gamage, Thomas Heidlauf, et al. Opencmiss: a multi-physics & multi-scale computational infrastructure for the vph/physiome project. Progress in biophysics and molecular biology, 107(1):32-47, 2011.